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Derivation of an eddy diffusivity coefficient depending on source distance for a shear dominated planetary boundary layer

I.P. Alves [a], G.A. Degrazia [a,*], D. Buske [b], M.T. Vilhena [c], O.L.L. Moraes [a], O.C. Acevedo [a]

[a] Departamento de Física, Universidade Federal de Santa Maria, Campus Universitário, Prédio 13 CCNE, 97105-900, Santa Maria/RS, Brazil
[b] Departamento de Matemática e Estatística, DME/IFM, Universidade Federal de Pelotas, Campus Universitário, CP 354, 96010-900, Pelotas/RS, Brazil
[c] Departamento de Engenharia Mecânica, Universidade Federal do Rio Grande do Sul, Sarmento Leite, 425, 3° andar, 90046-900, Porto Alegre/RS, Brazil

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ABSTRACT

In this study an integral and an algebraic formulation for the eddy diffusivities in a shear driven planetary boundary layer are derived for pollutant dispersion applications. The expressions depend on the turbulence properties and on the distance from the source. They are based on the turbulent kinetic energy spectra, Taylor's statistical diffusion theory and measured turbulent characteristics during intense wind events. The good agreement between the algebraic and the integral formulation for the eddy diffusivities corroborate the hypothesis that using an algebraic formulation as a surrogate for the eddy diffusivities in the neutral planetary boundary layer is valid. As a consequence, the vertical eddy diffusivity provided by the algebraic formulation and its asymptotic limit for large time (diffusion time much larger than the Lagrangian integral time scale), were introduced into an analytical air pollution model and validated against data from the classic Prairie Grass project. A statistical analysis, employing specific indices shows that the results are in good agreement with the observations. Furthermore, this study suggests that the inclusion of the memory effect, which is important in regions near to a continuous point source, improves the description of the turbulent transport process of atmospheric contaminants. Therefore, the major finding of this paper is the necessity of including the downwind distance-dependent eddy diffusivity for low continuous point sources in air quality modeling studies.

1. Introduction

The advection–diffusion equation has been extensively used in air pollution models to simulate mean concentrations of contaminants in the planetary boundary layer (PBL) [1,2]. Therefore, it is possible to construct a theoretical model for the dispersion from a continuous point source from an Eulerian perspective, given adequate boundary and initial conditions and the knowledge of the mean wind velocity field and of the concentration turbulent fluxes. The choice of an appropriate parameterization for such fluxes plays an important role in air quality dispersion models based on the advection–diffusion equation, so that much of the research on scalar dispersion concerns their specification.

The most commonly used scheme for closing the advection–diffusion equation is based on relating the turbulent concentration fluxes to the mean gradients through eddy diffusivities, which must carry within them the physical structure of the turbulent transport phenomenon (the K-theory). For a continuous point source, such eddy diffusivities may be a function

* Corresponding author.
E-mail addresses: ipmalves@gmail.com (I.P. Alves), gervasiodegrazia@gmail.com, degrazia@ccne.ufsm.br (G.A. Degrazia), danielabuske@pq.cnpq.br (D. Buske), vilhena@pq.cnpq.br (M.T. Vilhena), osvaldo.moraes@pq.cnpq.br (O.L.L. Moraes).

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of space and of the contaminant travel time [3]. Taylor's statistical diffusion theory (1921) indicates that turbulent dispersion depends on the proximity to a continuous point source, so that near the source the fluid particles retain the memory from their initial turbulent environment, while for long travel times such memory is lost. In this case, the particles motion depends only on the local turbulence properties [4].

The aim of this study is to propose a new formulation for the eddy diffusivities as a function of distance (travel time) from the source in inhomogeneous mechanical turbulence. It is based on the specification of the turbulent velocity spectra and on the statistical diffusion theory. Such eddy diffusivities, derived for neutral conditions are described by a complex integral formulation, which is numerically solved. They contain characteristic velocity and space scales of the energy-containing eddies and can describe the dispersion process when the scale of the plume is smaller than the turbulence scale, which covers the near and intermediate ranges from a continuous point source.

An additional aim of this work is to obtain a simple algebraic expression for the eddy diffusivities in a neutral PBL, which depends on the turbulence properties (inhomogeneous turbulence) and on the distance from the source. Therefore, the hypothesis to be tested in this study is whether the complex integral formulation for eddy diffusivities can be expressed by a simpler algebraic expression. Finally, the influence of retaining the memory effect in the turbulent dispersion process from a low continuous point source is investigated. To do so, a vertical eddy diffusivity that is function of the distance from the source is compared to its asymptotic limit employing an Eulerian air pollution model and analyzing how they reproduce observations from atmospheric dispersion experiments carried out in strong wind conditions [5].

2. Derivation of eddy diffusivities

2.1. Integral formulation

An important problem in physics of the turbulent transport is to understand how the turbulent kinetic energy (TKE) is distributed among the different eddy motion scales (frequencies). From a theoretical point of view, it is important to select the scales (frequencies) associated with the energy-containing eddies. These special eddies contain most of the TKE, playing a major part on PBL dispersion. Therefore, to establish a close relationship between the dispersion process and the frequencies of eddy motion, it is appropriate to introduce the formulation for the dispersion parameter σ_α, as given by Pasquill and Smithl [6];

$$\sigma_\alpha^2 = \frac{\sigma_i^2 \beta_i^2}{\pi^2} \int_0^\infty F_i^E(n) \frac{\sin^2(\pi n t/\beta_i)}{n^2} \mathrm{d}n, \tag{1}$$

where $\alpha = x, y, z$ and $i = u, v, w$, $F_i^E(n)$ is the Eulerian energy spectrum normalized by the Eulerian velocity variance σ_i^2, β_i is the ratio between the Lagrangian and Eulerian integral timescales, n is the frequency and t is the travel time.

The present model basically hinges on the Ref. [4] time-dependent equation for the evolution of the eddy diffusivities K_α,

$$K_\alpha = \frac{1}{2} \frac{\mathrm{d}\sigma_\alpha^2}{\mathrm{d}t}, \tag{2}$$

which says that the eddy diffusivity is the temporal derivative of the spatial variance. From Eqs. (1) and (2), we obtain

$$K_\alpha = \frac{\sigma_i^2 \beta_i}{2\pi} \int_0^\infty \frac{F_i(n) \sin(2\pi n t/\beta_i)}{n} \mathrm{d}n. \tag{3}$$

As Eq. (1) is described in terms of β_i, it also represents σ_α^2 from a Lagrangian perspective and thus Eq. (3) determines a Lagrangian eddy diffusivity K_α in terms of the ratio of the Eulerian energy spectrum to the Eulerian velocity variance as the kernel of a Fourier transform in frequency space.

The Eulerian velocity spectra under neutral conditions can be described as a function of shear driven PBL scales as Ref. [7]:

$$\frac{nS_i(n)}{\mu_*^2} = \frac{1.5 C_i \Phi_\varepsilon^{2/3} f}{\left[1 + \frac{1.5 f^{5/3}}{(f_m)_i^{5/3}}\right] (f_m)_i^{5/3}}, \tag{4}$$

where $C_i = \alpha_i(0.50 \pm 0.02)(2\pi\kappa)^{-2/3}$; $\alpha_i = 1, 4/3$ and $4/3$ for the u, v and w components respectively [8]; $\kappa = 0.4$ is the von Karman constant, $f = nz/U$ is the dimensionless frequency (n being the cyclic frequency, U the mean horizontal wind speed and z the observation height), $(f_m)_i$ is the dimensionless frequency of the neutral spectral peak and $\mu_*^2 = (\mu_{*0})^2[1 - (z/h)]^{1.7}$ is the local friction velocity for a neutral PBL [7] with μ_{*0} being the surface friction velocity and h is the depth of the neutral PBL. The dimensionless dissipation rate is defined as $\Phi_\varepsilon = \kappa z \varepsilon / (u_*)_0^3$ where ε is the mean TKE dissipation per unit time per unit mass of fluid, and its magnitude depends only on quantities that characterize the energy-containing eddies. The above α_i values are derived from the turbulence isotropy in the inertial subrange of the energy spectrum.

The analytical integration of Eq. (4) over the whole frequency domain leads to the Eulerian turbulent velocity variance

$$\sigma_i^2 = \frac{1.5zC_i\Phi_\varepsilon^{2/3}u_*^2}{U\,(f_m)_i^{5/3}}\int_0^\infty \frac{\mathrm{d}n}{\left[1+1.5\left(\frac{nz}{U(f_m)_i}\right)^{5/3}\right]} \tag{5}$$

and

$$\sigma_i^2 = \frac{2.32C_i\Phi_\varepsilon^{2/3}u_*^2}{(f_m)_i^{2/3}} \tag{6}$$

which is used to normalize the spectrum so that the normalized Eulerian spectrum can be written as:

$$F_i^E = \frac{S_i(n)}{\sigma_i^2} = \frac{0.64\frac{z}{U}}{(f_m)_i}\left\{1+1.5\left(\frac{nz}{U(f_m)_i}\right)^{5/3}\right\}^{-1}. \tag{7}$$

Substituting Eqs. (6) and (7) into Eq. (3), and considering [9–12], yields

$$K_\alpha = \frac{0.085C_i^{1/2}\Phi_\varepsilon^{1/3}u_*z}{(f_m)_i^{4/3}}\int_0^\infty \frac{\mathrm{sen}(an)\mathrm{d}n}{n\left\{1+1.5\left(\frac{nz}{U(f_m)_i}\right)^{5/3}\right\}}. \tag{8}$$

The following terms from Eq. (3) are written as

$$\frac{\sigma_i^2\beta_i}{2\pi} = \frac{0.13UC_i^{1/2}\Phi_\varepsilon^{1/3}u_*}{(f_m)_i^{1/3}},$$

$$\frac{2\pi t}{\beta_i} = a = \frac{17.4C_i^{1/2}\Phi_\varepsilon^{1/3}}{(f_m)_i^{1/3}}\frac{z}{U}\frac{Xu_*}{Uz}$$

where a time to space transposition is applied to the time dependency in Eq. (3) to yield a spatially dependent K_α, with $X' = Xu_*/Uz$ being a dimensionless distance defined by the ratio of travel time X/U to the shear turbulent timescale z/μ_*. Defining $n' = bn$ where $b = \left[\frac{1.5}{(f_m)_i^{5/3}}\right]^{3/5}\frac{z}{U}$, Eq. (8) can be written as

$$K_\alpha = \frac{0.085C_i^{1/2}\Phi_\varepsilon^{1/3}u_*z}{(f_m)_i^{4/3}}\int_0^\infty \frac{\mathrm{sen}\left(an'/b\right)}{\left[1+(n')^{5/3}\right]}\frac{\mathrm{d}n'}{n'}, \tag{9}$$

which expands to

$$\frac{K_\alpha}{u_*h} = \frac{0.085C_i^{1/2}\Phi_\varepsilon^{1/3}\frac{z}{h}}{(f_m)_i^{4/3}}\int_0^\infty \frac{\mathrm{sen}\left[13.64C_i^{1/2}\Phi_\varepsilon^{1/3}\,(f_m)_i^{2/3}X'n'\right]\mathrm{d}n'}{\left[1+(n')^{5/3}\right]n'}. \tag{10}$$

The generalized eddy diffusivity as a function of downwind distance (Eq. (10)) is dependent on z and yields a description of the turbulent dispersion process in the near, intermediate, and far ranges from a continuous point source, with the memory effect of the turbulent transport being considered.

2.2. Algebraic formulation

The following simple algebraic relation has been largely used to fit observed dispersion parameters in the PBL under different stability conditions [13–17]:

$$\sigma_\alpha = \frac{\sigma_i t}{\left[1+\frac{1}{2}\left(t/T_{Li}\right)\right]^{1/2}}. \tag{11}$$

In Eq. (11), T_{Li} is the Lagrangian decorrelation time scale. For non-homogeneous turbulence, such decorrelation time scales can be expressed as Ref. [12]:

$$T_{L_i} = \frac{\beta_i F_i^E(n\to 0)}{4}. \tag{12}$$

Therefore, in neutral conditions, the local decorrelation time scales can be derived from Eqs. (12) and (7) as

$$T_{L_i} = 0.088 \frac{z}{\sigma_i (f_m)_i}. \tag{13}$$

A formulation for the algebraic time dependent eddy diffusivity can be obtained from Eqs. (2) and (11), yielding

$$K_\alpha = \frac{\sigma_i^2 t}{\left(1 + \frac{t}{2T_{Li}}\right)^2} \left(1 + \frac{t}{4T_{Li}}\right). \tag{14}$$

Eqs. (3) and (14) are identical for small and large travel times. As a consequence, Eq. (14) can be utilized to generate a simple algebraic expression that can be used as a surrogate of Eq. (3). Thus, substituting from Eqs. (6) and (13) into algebraic expression (14), an eddy diffusivity depending on the source distance can be written as

$$\frac{K_\alpha}{u_* h} = \frac{0.135 C_i \Phi_\varepsilon^{2/3} X' \frac{z}{h} \left[0.232 + (f_m)_i^{2/3} C_i^{1/2} \Phi_\varepsilon^{1/3} X'\right]}{(f_m)_i^{2/3} \left[0.116 + (f_m)_i^{2/3} C_i^{1/2} \Phi_\varepsilon^{1/3} X'\right]^2}. \tag{15}$$

The asymptotic behavior of Eqs. (3) and (14) for large diffusion travel times when the eddy diffusivity has lost its memory from the initial conditions, therefore depending only on flow properties is Ref. [18]

$$K_\alpha = \frac{\sigma_i^2 \beta_i F_i(0)}{4}, \tag{16}$$

this expression, along with $\beta_i = 0.55U/\sigma_i$ and Eqs. (6) and (7) leads to

$$\frac{K_\alpha}{u_* h} = \frac{0.134 C_i^{1/2} \Phi_\varepsilon^{1/3} \frac{z}{h}}{(f_m)_i^{4/3}}. \tag{17}$$

The turbulent parameters $(f_m)_i$ and Φ_ε must be inferred from field observations at a shear-dominated PBL. For the neutral case, the spectral peak frequency $(f_m)_i$ describes the spatial and temporal characteristic scales of the energy-containing eddies, and can be expressed as Refs. [7,19–21]:

$$(f_m)_i = (f_m)_{0i} \left[1 + 0.03 a_i \frac{f_c z}{\mu_{*0}}\right], \tag{18}$$

where $(f_m)_{0i}$ is the spectral peak frequency at the surface, $f_c = 10^{-4} s^{-1}$ is the Coriolis parameter, and $a_u = 3889$, $a_v = 1094$ and $a_w = 500$ [7].

Although the energy dissipation rate ε is ultimately due to the fluid viscosity and occurs at the smallest eddies, it may be expressed in terms of scales that characterize the energy-containing eddies [22]. Therefore, it is natural that the eddy diffusivities are described in terms of Φ_ε.

In the present study, the values of Φ_ε and of the spectral peak frequencies $(f_m)_i$ have been measured during a meteorological phenomenon known as north wind flow (NWF), which occurs in a regional scale at the center of Rio Grande do Sul state, in southern Brazil [21]. The atmospheric synoptic conditions associated with the NWF cases are characterized by intense mean wind speeds, so that the large vertical wind shear was produced predominantly by mechanical turbulence. Therefore, one of the main peculiarities of the present turbulent parameterization (values of $(f_m)_i$ and Φ_ε obtained from the NWF cases) is that it regards the turbulent dispersion in neutral situations. For a more detailed discussion about the turbulence measurements taken during NWF events we suggest the paper by Arbage et al. [21]. The observations indicate that the mean values of $(f_m)_i$ are [21]: $(f_m)_{0u} = 0.04$, $(f_m)_{0v} = 0.1$ and $(f_m)_{0w} = 0.33$, which are in fair agreement with those obtained at the classic Kansas and Minnesota micrometeorological experiments [23]. At neutral stability atmospheric condition it is expected that Φ_ε approaches unity, due to the balance between shear production and viscous turbulence dissipation in the absence of any buoyant production and transport. Thus the value of $\Phi_\varepsilon = 1.1$ obtained from the inertial subrange of the vertical velocity spectra is in good agreement with Kansas results [21,24] and with theoretical predictions [21,24,25]. At this point it is important to note that the role of the NWF data, in the present analysis, is that of providing the values of $(f_m)_i$ and Φ_ε for Eqs. (10), (15) and (17). For large winds, such as those occurring during NWF cases, a neutral stability state in the PBL can be considered. Thus, for strong winds, mechanical turbulent forcing balances and dominates the thermal effects and consequently the real PBL can be assumed in a neutral condition.

For a neutral stability situation, characterized by large wind speeds, the turbulent transport of scalar and vector species occurs mainly in the vertical direction. Therefore, this analysis will focus on the vertical eddy diffusivities. To proceed, the vertical eddy diffusivities can be obtained from Eqs. (10), (15) and (18) as a function of both the downwind distance X' and

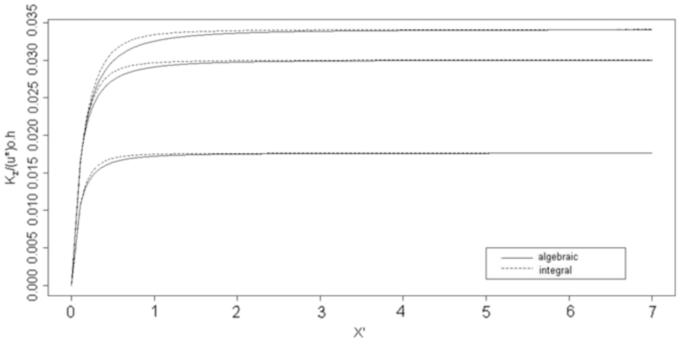

Fig. 1. Normalized eddy diffusivity $K_z/u_{*0}.h$ from integral (Eq. (20)) and algebraic (Eq. (21)) formulations. From top to bottom the dimensionless heights are $z/h = 0.25, 0.50, 0.75$.

of the height z using $C_w = 0.36$, $(f_m)_i = 0.33$ and $\Phi_\varepsilon = 1.1$ and [21,26,27]:

$$h = \frac{0.2u_{*0}}{f_c}, \tag{19}$$

$$\frac{K_z}{u_{*0}h} = \frac{0.23\frac{z}{h}\left(1-\frac{z}{h}\right)^{0.85}}{\left(1+3.00\frac{z}{h}\right)^{4/3}} \int_0^\infty \frac{\operatorname{sen}\left[4.03\left(1+3.00\frac{z}{h}\right)^{2/3} n'X'\right] dn'}{\left[1+(n')^{5/3}\right] n'} \tag{20}$$

and

$$\frac{K_z}{u_{*0}h} = \frac{0.11\frac{z}{h}\left(1-\frac{z}{h}\right)^{0.85} X'\left[0.23+0.30\left(1+3.00\frac{z}{h}\right)^{2/3} X'\right]}{\left(1+3.00\frac{z}{h}\right)^{2/3}\left[0.12+0.30\left(1+3.00\frac{z}{h}\right)^{2/3} X'\right]^2}. \tag{21}$$

Fig. 1 shows the eddy diffusivities $K_z/u_{*_0}h$ as given by the integral (Eq. (20)) and algebraic (Eq. (21)) formulations for three different heights ($z/h = 0.25, 0.50, 0.75$). For a given height, the eddy diffusivities given by both Eqs. (20) and (21) are initially zero, increasing at first linearly with X', then more slowly, and finally tending to a constant value that can be obtained from Eqs. (17), (18) with $(f_m)_{0w} = 0.33$, $C_w = 0.36$ and $\Phi_\varepsilon = 1.1$. Such an expression, appropriate for far source distance reads as

$$\frac{K_z}{u_{*0}h} = \frac{0.37\frac{z}{h}\left(1-\frac{z}{h}\right)^{0.85}}{\left(1+3.00\frac{z}{h}\right)^{4/3}}. \tag{22}$$

Fig. 1 shows a large agreement between the algebraic and integral eddy diffusivity formulations for all vertical levels considered. This fact indicates that the turbulent dispersion parameterization given by a simple algebraic interpolation can accurately represent the diffusion in both the near and intermediate ranges from a continuous point source.

3. An analytical air pollution model

The advection–diffusion equation for air pollution dispersion in the atmosphere is essentially a statement of conservation of the suspended material, being written as:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = -\frac{\partial \overline{u'c'}}{\partial x} - \frac{\partial \overline{v'c'}}{\partial y} - \frac{\partial \overline{w'c'}}{\partial z} + S \tag{23}$$

where $\bar{c}$ denotes the average concentration of a passive contaminant, $\bar{u}$, $\bar{v}$, $\bar{w}$ are the mean wind components along the x, y and z axis, respectively, and S is the source term. The terms $\overline{u'c'}$, $\overline{v'c'}$ and $\overline{w'c'}$ represent, respectively, the turbulent fluxes of contaminants in the longitudinal, cross-wind and vertical directions.

Eq. (23) has four unknown variables (the concentration $\bar{c}$ and the three turbulent fluxes), which leads us to the well-known turbulence closure problem. One of the most widely used closures for Eq. (23), also known as K-theory, is based on the gradient transport hypothesis and, in analogy with Fick's law of molecular diffusion, consists in assuming that turbulence causes a net motion of a given quantity down the gradient of that quantity, at a rate that is proportional to the gradient [28]:

$$\overline{u'c'} = -K_x\frac{\partial \bar{c}}{\partial x}; \qquad \overline{v'c'} = -K_y\frac{\partial \bar{c}}{\partial y}; \qquad \overline{w'c'} = -K_z\frac{\partial \bar{c}}{\partial z} \tag{24}$$

where K_x, K_y, K_z are the Cartesian components of the eddy diffusivity in the x, y and z directions, respectively. In a first order closure, such as the one assumed here, all the information on the turbulence complexity is contained within the eddy diffusivities.

Substituting expressions (24) in Eq. (23), the advection–diffusion equation may be rewritten as Ref. [29]:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial \bar{c}}{\partial z}\right) + S. \tag{25}$$

K-theory is widespread used as the mathematical basis for simulating air pollution dispersion. However, such closure has intrinsic limits. It works well when the dimension of the dispersed material is much larger than the size of the turbulent eddies involved in the diffusion process. Besides, the down-gradient transport hypothesis is inconsistent with observed features of turbulent diffusion in the upper portion of the mixed layer [30]. Despite these well known limitations, K-closure is largely used in several atmospheric conditions because:

(i) it describes the diffusive transport in an Eulerian framework, easily comparable to the majority of the existent measurements, which are also obtained from an Eulerian perspective;
(ii) it produces results that agree with experimental data as well as any other more complex models;
(iii) it is not as computationally expensive as higher order closures usually are.

The advection–diffusion equation (25) can be solved analytically by the 3D-GILTT approach [31,32]. Here, to allow comparison with experimental data and to use the parameterization obtained for the NWF (Eqs. (21) and (22)) some assumptions are taken at the advection–diffusion equation (25): stationarity, a Cartesian coordinate system in which x direction coincides with that one of the predominant wind (so it is derived the longitudinal wind), the advection is much larger than the diffusion in the x-direction and the cross-wind integration of the Eq. (25). With such considerations, the problem is simplified to:

$$\bar{u}\frac{\partial \overline{c_y}}{\partial x} = \frac{\partial}{\partial z}\left(K_z\frac{\partial \overline{c_y}}{\partial z}\right), \tag{26}$$

here $\overline{c_y}$ represents the average cross-wind integrated concentration, for $0 < z < h$ and $x > 0$, subject to the boundary conditions of zero flux at the ground and PBL top (h), and assuming the existence of a source with emission Q at height H_s:

$$K_z\frac{\partial \overline{c_y}}{\partial z} = 0 \quad \text{at } z = 0, h, \tag{26a}$$

$$\bar{u}\overline{c_y} = Q\delta(z - H_s) \quad \text{at } x = 0 \tag{26b}$$

where δ is the generalized Dirac delta function.

Following Refs. [31,33], it is posed that the solution of problem (26) has the form:

$$\overline{c_y}(x, z) = \sum_{n=0}^{N} \bar{c}_n(x)\Psi_n(z) \tag{27}$$

where $\Psi_n(z)$ are the eigenfunctions of the associated Sturm–Liouville problem, or $\Psi_n(z) = \cos(\lambda_n z)$ where $\lambda_n = n\pi/h$ ($n = 0, 1, 2, \ldots$) are the respective eigenvalues.

To determine the unknown coefficient $\bar{c}_n(x)$, Eq. (27) is substituted in Eq. (26) and the operator $\int_0^h ()\Psi_m(z)\mathrm{d}z$ is applied, leading to:

$$-\sum_{n=0}^{N} \bar{c}_n'(x)\int_0^h \bar{u}\Psi_n\Psi_m \mathrm{d}z - \sum_{n=0}^{N} \bar{c}_n(x)\lambda_n^2\int_0^h K_z\Psi_n\Psi_m \mathrm{d}z + \sum_{n=0}^{N} \bar{c}_n(x)\int_0^h K_z'\,\Psi_n'\Psi_m\,\mathrm{d}z = 0, \tag{28}$$

which can be recast in a matrix form as:

$$Y'(x) + FY(x) = 0, \tag{29}$$

subject to the condition:

$$Y(0) = \bar{c}_n(0). \tag{29a}$$

Here, $Y(x)$ is the vector whose components are $\bar{c}_n(x)$ and $F = B^{-1}\cdot E$; $B = \{b_{n,m}\}$ and $E = \{e_{n,\mathrm{m}}\}$ are the matrices whose entries are respectively:

$$b_{n,m} = -\int_0^h \bar{u}\Psi_n\Psi_m \mathrm{d}z \quad \text{and} \quad e_{n,m} = \int_0^h K_z'\Psi_n'\Psi_m \mathrm{d}z - \lambda_n^2\int_0^h K_z\Psi_n\Psi_m \mathrm{d}z. \tag{29b}$$

For the source condition (Eq. (26b)), a similar procedure leads to:

$$\bar{c}_n(0) = Q\Psi_m(H_s)A^{-1}, \tag{30}$$

where A^{-1} is the inverse matrix of A given by

$$a_{n,m} = \int_0^h \bar{u}\Psi_n(z)\Psi_m(z)\mathrm{d}z. \quad (31)$$

Finally, the transformed problem represented by Eq. (29) can be solved analytically using the Laplace Transform technique and diagonalization of the matrix $F = X\,D X^{-1}$ [33], leading to:

$$\overline{Y(s)} = X\,(sI + D)^{-1}\,X^{-1}Y(0) \quad (32)$$

where $\overline{Y(s)}$ denotes the Laplace Transform of vector $Y(x)$. Here, X is the eigenvectors matrix of matrix F and X^{-1} is its inverse. Matrix D is the diagonal matrix of the eigenvalues of matrix F and the entry of matrix $(sI + D)$ has the form $\{s + d_n\}$. Performing the Laplace transform inversion of Eq. (32), it leads to:

$$Y(x) = X \cdot G(x) \cdot \xi \quad (33)$$

where $G(x)$ is the diagonal matrix with components $\mathrm{e}^{-d_n x}$ and ξ ($\xi = X^{-1}P(0)$) is found from equation $X\xi = Y(0)$. Their values are calculated by LU decomposition, which has a smaller computational cost than a matrix inversion [34].

Finally, using the formula of the inverse (27), $\overline{c_y}(x, z) = \sum_{n=0}^{N} \bar{c}_n(x)\Psi_n(z)$, it is possible to write the final two-dimensional solution for problem (26), where $\Psi_n(z) = \cos(\lambda_n z)$ and $\bar{c}_m(x, z)$ arises from the solution of the transformed problem (Eq. (29)), being given by Eq. (33).

4. Model evaluation

In this section, the eddy diffusivities derived in Section 2 (Eqs. (21) and (22)) are introduced in the GILTT model (Eq. (27)), with the purpose of evaluating the performance of the solution in reproducing experimentally observed ground-level concentrations. To do that, SO_2 tracer data concentrations from the Prairie Grass dispersion experiment carried in O'Neill, Nebraska, in 1956, will be considered

In that experimental campaign, contaminants (SO_2) were emitted without buoyancy from a 0.46 m height and sampled at a height of 1.5 m at five downwind distances (50, 00, 200, 400, 800 m) [35]. The Prairie Grass site was flat with a 0.6 cm roughness length. From the Prairie Grass runs, thirteen cases in which the mean wind speed was greater than 6.0 ms^{-1} with values of $(u_*)_0 \geq 0.4\ \mathrm{ms}^{-1}$ were selected. Table 1 provides the values of the micrometeorological parameters for the selected Prairie Grass runs. The values of $\bar{u}$ and $(u_*)_0$ expressed in Table 1, are characteristic of a neutral PBL [27]. Therefore, the turbulent parameters (Φ_ε and $(f_m)_i$), obtained for a neutral PBL from NWF data (strong wind velocity cases), can be used in Eqs. (21) and (22) to simulate the measured concentrations for these selected neutral Prairie Grass experiments.

The wind speed profile used in the simulations follows a power law, being expressed as Ref. [26]:

$$\frac{\bar{u}_z}{\bar{u}_1} = \left(\frac{z}{z_1}\right)^n, \quad (34)$$

where $\bar{u}_z$ and $\bar{u}_1$ are the mean horizontal wind speeds at heights z and z_1, while $n = 0.1$ is an exponent related to the turbulence intensity [36]. In Table 1, the measured and computed ground-level cross-wind concentrations from the GILTT model employing the eddy diffusivities given by Eqs. (21) and (22) are presented.

The performance of the GILTT model with the eddy diffusivities given by Eqs. (21) and (22) are shown in Table 2 and Fig. 2. Table 2 exhibits the result of the statistical analysis that compares observed and predicted values of ground-level cross-wind integrated concentration (Cy). The statistical indices in Table 2 are suggested by Hanna and Paine [37] and defined as:

$$\mathrm{NMSE\ (normalized\ mean\ square\ error)} = \overline{(C_o - C_p)^2}/\overline{C_p C_o},$$

$$\mathrm{FA2} = \text{fraction of data (\%, normalized to 1) for } 0.5 \leq (C_p/C_o) \leq 2,$$

$$\mathrm{COR\ (correlation\ coefficient)} = \overline{(C_o - \overline{C_o})(C_p - \overline{C_p})}/\sigma_o\sigma_p,$$

$$\mathrm{FB\ (fractional\ bias)} = \overline{C_o} - \overline{C_p}/0.5(\overline{C_o} + \overline{C_p}),$$

$$\mathrm{FS\ (fractional\ standard\ deviations)} = (\sigma_o - \sigma_p)/0.5(\sigma_o + \sigma_p)$$

where C is concentration and the subscripts o and p refer to the observed and predicted values, respectively, and where overbars indicate averages. The statistical index FB indicates whether the predicted quantities underestimate or overestimate the observed ones. The statistical index NMSE represents the quadratic error of the predicted quantity in relation to the observed one. The index FS indicates a comparison between predicted and observed plume spreading. The index FA2 provides the fraction of data for which $0.5 \leq C_p/C_o \leq 2$. Better results lead to values of NMSE, FB and FS that approach zero, while COR and FA2 approach unity in the same case. Fig. 2 shows the scatter diagram between observed and predicted ground-level crosswind integrated concentrations for the Prairie Grass concentrations data set.

Table 2 and Fig. 2 show that the GILTT model employing the turbulence parameterizations given by Eqs. (21, memory-containing eddy diffusivity) and (22, asymptotic eddy diffusivity), simulate quite well the experimental concentration data

Table 1
Meteorological parameters and ground-level crosswind integrated concentrations measured during the Prairie Grass experiment [5] (first line) and simulated by the GILTT method for Eqs. (22) and (21) (second and third lines, respectively).

Run	h (m)	$(u_*)_0$ (ms^{-1})	$\bar{u}_{10\ m}$ (ms^{-1})	Q (gs^{-1})	50 m (gm^{-2})	100 m (gm^{-2})	200 m (gm^{-2})	400 m (gm^{-2})	800 m (gm^{-2})
					3.30	1.80	0.81	0.29	0.092
5	780	0.40	7.0	78	3.16	2.01	0.95	0.30	0.24
					3.80	2.02	1.21	0.35	0.10
					3.70	2.20	1.00	0.41	0.13
9	550	0.48	8.4	92	3.49	2.25	1.11	0.40	0.29
					4.38	2.59	1.57	0.48	0.14
					4.50	2.20	0.86	0.27	0.058
19	650	0.41	7.2	102	4.30	2.74	1.33	0.45	0.36
					5.29	2.96	1.79	0.54	0.16
					3.40	1.80	0.85	0.34	0.13
20	710	0.63	11.3	102	2.68	1.71	0.83	0.26	0.21
					3.26	1.80	1.09	0.32	0.09
					3.90	2.20	1.04	0.39	0.127
26	900	0.45	7.8	98	3.33	2.12	0.99	0.29	0.24
					3.33	2.01	1.22	0.35	0.10
					4.30	2.30	1.16	0.46	0.176
27	1280	0.44	7.6	99	2.82	1.84	0.81	0.24	0.20
					3.18	2.11	0.92	0.25	0.07
					4.20	2.30	1.11	0.40	0.10
30	1560	0.48	8.5	98	2.20	1.47	0.63	0.17	0.15
					2.41	1.58	0.67	0.18	0.05
					5.00	2.40	1.09	0.37	0.12
43	600	0.40	6.1	99	4.80	3.01	1.48	0.54	0.39
					6.14	3.54	2.07	0.59	0.19
					4.50	2.30	1.09	0.43	0.14
44	1450	0.42	7.2	101	2.79	1.85	0.80	0.22	0.19
					3.09	2.04	0.87	0.24	0.19
					4.30	2.40	1.16	0.45	0.15
49	550	0.47	8.0	102	4.02	2.59	1.28	0.47	0.34
					5.09	3.00	1.81	0.51	0.16
					4.20	2.30	0.91	0.39	0.11
50	750	0.46	8.0	103	3.71	2.36	1.13	0.36	0.29
					4.47	2.42	1.45	0.42	0.12
					4.70	2.40	1.00	0.38	0.084
51	1880	0.47	8.0	102	2.10	1.43	0.59	0.16	0.14
					2.26	1.46	0.61	0.17	0.05
					3.50	2.10	1.14	0.53	0.20
61	450	0.53	9.3	102	3.65	2.40	1.22	0.44	0.34
					4.70	3.01	1.83	0.54	0.17

Table 2
Statistical indices evaluating the model performance.

Model	NMSE	COR	FA2	FB	FS
GILTT Eq. (22)	0.15	0.93	0.86	0.11	0.18
GILTT Eq. (21)	0.16	0.91	0.89	−0.02	−0.04

for the neutral Prairie Grass tracer experiments. The statistical analysis shows that all indices are within the acceptable range, with NMSE, FB and FS magnitudes being relatively close to zero and COR and FA2 approaching the value of 1.0. Furthermore, it is worth to notice that FB and FS given by the GILTT model using K_z varying with the distance from the source is five times smaller than those obtained from the GILTT model utilizing the asymptotic K_z. This result indicates that it is relevant to include the downwind distance-dependent eddy diffusivity in air quality modeling studies.

5. Conclusions

A general development to obtain eddy diffusivities that depend on source distance for a shear driven turbulent PBL has been proposed. The approach is based on a model for the turbulent kinetic energy spectra and on Taylor statistical diffusion theory. The derived eddy diffusivities are valid in the near, intermediate, and far ranges from a continuous point source.

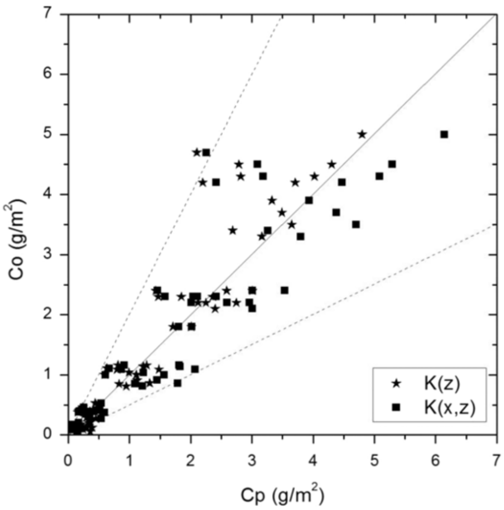

Fig. 2. Comparison between observed (C_o) and predicted (C_p) concentrations for the Prairie Grass experiment. Lines indicate a factor of two ($C_0/C_p \epsilon [0.5; 2]$).

Employing turbulent parameters that were measured during an intense wind phenomenon known as north wind flow [21] the current model provides an integral formulation for the vertical eddy diffusivity that depends on the distance from the source for inhomogeneous turbulence in a neutral PBL. Such vertical eddy diffusivities, calculated from a complex integral, have been compared to a simpler algebraic formulation. Therefore, the algebraic formulation was introduced in an analytical air pollution model, and compared to concentration data from the classic Prairie Grass experiments. The Prairie Grass selected runs employed in this work were accomplished in a neutral PBL. Therefore, the relevant role of the north wind measurements in this study is those of supply magnitudes of $(f_m)_w$ and Φ_ε for a neutral PBL. These values were used to obtain Eqs. (20)–(22). This explains the importance of the north wind data in the present analysis and their connection with the Prairie Grass neutral experimental runs.

The performance of the dispersion model using the algebraic formulation evaluated by specific statistical indices shows a good degree of agreement between the algebraic and integral formulations. Furthermore, to evaluate the memory effect, and therefore to establish confidence in the parameterization shown in Eq. (21), the results from a simulation utilizing the asymptotic vertical eddy diffusivity (Eq. (22)), valid for large diffusion travel times, are also compared to the Prairie Grass observations. The scatter diagram (Fig. 2) and the statistical indices (Table 2) show a good agreement between the modeled results and the experimental ones. Specifically, the statistical indices FB and FS allow concluding that the results obtained with the eddy diffusivity that depends on source distance (Eq. (21)) are better than those reached using an asymptotic eddy diffusivity (Eq. (22)), valid only for the far range from a continuous point source. Therefore, the current analysis suggests that the inclusion of the memory effect in the eddy diffusivity, improves the description of the turbulent transport of atmospheric contaminants released from a low continuous point source. At this point, it is important to mention that for elevated continuous point source, [3] have already shown that the use of a distance-dependent eddy diffusivity in air quality modeling improves the simulations over the use of an asymptotic eddy diffusivity. Thus, that result and the present investigation show that the retention of the memory effect in the eddy diffusivity formulation is important for the simulation of contaminant turbulent diffusion for both low and elevated continuous point sources.

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